Wavelength calibration of a monochromator system

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Abstract. A new system for measurement of spectral power responsivity of detectors, utilising a monochromator system, was implemented at NMISA and characterised. The monochromator system includes sources of optical radiation, input optics, order sorting filters, a scanning double monochromator, diffraction gratings and output optics. As part of the characterisation, wavelength calibrations were performed in the wavelength regions of 200 nm to 400 nm and 600 nm to 1 100 nm. This was done by measuring the relevant spectral lines of wavelength standards selected from the NIST Atomic Spectra Database, and applying corrections for ambient conditions using the Engineering Metrology Toolbox of NIST. The monochromator steps corresponding to the spectral peaks measured were determined using the steep-side method. A linear fit of the spectral peaks versus the corresponding monochromator steps provided the wavelength calibration equations. These were then used when scanning the wavelength regions with the monochromator software. Uncertainty of measurement analyses were performed for each of the wavelength calibrations to determine the uncertainty associated with the wavelength position of the monochromator and its influence on the spectral power responsivity of a detector.

1. Introduction

A new system for measurement of spectral power responsivity of detectors was implemented at NMISA. This measurement system consists of a scanning double monochromator and other components selected based on the system's requirements. For this measurement system where a low uncertainty of measurement is required, it is critical to have good wavelength accuracy of the double monochromator. In this case, a double monochromator should be calibrated for wavelength before any measurement is performed and with each change in the monochromator setup, such as a change in diffraction gratings. This is done to determine the true position of the wavelength spectrum with an associated uncertainty. The wavelength calibration produces a wavelength calibration equation, which may be used by the monochromator software when scanning through a wavelength region to record data.

A wavelength calibration is performed with spectral line sources used as wavelength standards. These are lamps that contain specific elements and through electrical discharge in such a gas or vapour, emissions lines occur at known wavelengths [1]. The NIST Atomic Spectra Database [2] lists the wavelengths of these emissions and also indicates the stronger emission spectral lines. Figure 1 provides an example of the emission spectral lines of the argon spectral line source used in the wavelength region of 600 nm to 1 100 nm.

2. Determining the wavelength calibration equation

The appropriate spectral line source should be selected for the wavelength region in which the calibration is to be performed. At first, a large spectral area scan should be performed to determine which spectral lines to use, as shown in Figure 1. Good spectral lines will be those free of line blending. Spectral lines that are in the noise level should also be avoided. At least three spectral lines should be selected in the wavelength region to be measured to provide sufficient data for a good statistical fit. For a monochromator system with symmetric bandpass, the wavelength of the peak of the spectral line may be determined using the steep-side method described in Kostkowski [1]. This method determines the wavelength of the peak of the spectral line by averaging the wavelengths at the steep sides of the spectral line at 10 % of the maximum signal, λ_1 and λ_2, refer to Figure 2. The wavelength of the peak or center wavelength is given by

$$\lambda_{\mathrm{c}} = \frac{\lambda_1 + \lambda_2}{2} \tag{1}$$

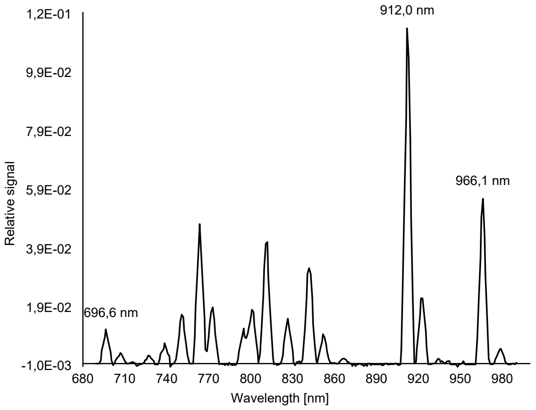

Figure 1. Emission spectral lines of the argon spectral line source used for the wavelength calibration in the visible to near-IR region.

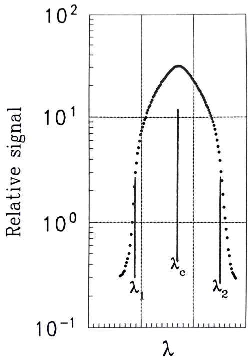

Figure 2. Excerpt from Kostkowski [1] demonstrating the steep-side method for a wavelength calibration.

The atomic emission spectral lines in vacuum should be corrected for ambient conditions. This may be done with the NIST Enigineering Metrology Toolbox [3] which utilises the modified Edlén equation to calculate the index of refraction of ambient air, n, from the supplied laboratory air temperature, relative humidity and air pressure. It calculates the wavelength in ambient air, λ_{air}, from the wavelength in vacuum, λ_{vac}, and the refractive index using the relationship:

$$\lambda_{air} = \frac{\lambda_{vac}}{n} \tag{2}$$

Once the spectral lines in ambient air are obtained, the monochromator steps versus the wavelength of the peak of each corrected spectral line are plotted. The appropriate fit for the data is derived to obtain the expected wavelength calibration equation.

3. Method

A wavelength calibration was performed for the double monochromator in the wavelength regions of 200 nm to 400 nm and 600 nm to 1 100 nm using the standard laboratory procedure. The relevant spectral line sources were used, together with a silicon photodiode detector and a variable gain low noise current amplifier connected to a multimeter operated with the monochromator software. The spectral lines were obtained from the NIST Atomic Spectra Database. To find the monochromator steps corresponding to the peak wavelength of each spectral line, the steep-side method as described in Section 2 was used. The ambient conditions were measured during each calibration and a correction was applied for temperature, atmospheric pressure and relative humidity, to each spectral line wavelength using the Engineering Metrology Toolbox of NIST. A linear fit of the spectral peaks versus the corresponding monochromator steps provided the wavelength calibration equations.

Verification of the wavelength calibration equations obtained in each wavelength region was performed by calculating the corresponding monochromator steps and moving the scan controllers of the monochromator to the laser lines at 543 nm and 632,8 nm, respectively. The peak signal of each laser line was found at the monochromator position within the stated wavelength uncertainty.

Uncertainty analyses were performed based on JCGM 100:2008 (GUM) [4]. During calibration there are many factors that influence the measurement result and therefore contribute to the measurement uncertainty. These sources of uncertainty are called input quantities, X, or uncertainty contributors, and their estimates are combined to produce the uncertainty of measurement. An uncertainty calculation starts with the estimated uncertainty, $u_{\mathrm{e}}(x)$, of the value, x, of these input quantities or uncertainty contributors, each of which has a defined probability distribution with an associated coverage factor, k. From this, the standard uncertainty, $u(x)$, is calculated as the quotient of the estimate of the uncertainty contributor and the coverage factor. A sensitivity coefficient, c, may have to be obtained to determine the sensitivity of the standard uncertainty to its contribution to the combined uncertainty, due to a change in the input quantity. The contribution to the combined standard uncertainty, $u(y)$, is therefore calculated as the product of the standard uncertainty and the sensitivity coefficient. These contributions, $u(y)$, are appropriately combined to obtain the combined standard uncertainty, $u_{\mathrm{c}}(y)$. The expanded uncertainty, U, is reported and determined by multiplying the combined standard uncertainty with the appropriate coverage factor.

Several uncertainty contributors were considered and quantified for the wavelength calibrations performed in both wavelength regions. The complete uncertainty calculations on both wavelength regions are provided in Appendix A and Appendix B.

3.1. Wavelength region of 200 nm to 400 nm

A set of 1 200 g/mm ruled gratings blazed at 300 nm was installed in the double monochromator, and a mercury spectral line source was used. A large spectral area scan was performed with the monochromator from 233 nm to 552 nm in 1 nm intervals using a bandwidth of 5 nm. From this scan, the spectral lines used for this calibration were selected. These spectral lines, in vacuum, were 253,7283 nm, 296,8149 nm and 435,9560 nm. Each of these spectral lines were scanned three times using a smaller wavelength interval of 0,2 nm. The scans were performed over a wavelength range of ± 5 nm of the spectral line.

When 10 % of the maximum signal is calculated, there is not necessarily a signal measured at the scanning steps that matches this value. Instead of selecting the closest value of monochromator steps, a linear fit was used on each steep side of the spectral line. The recorded signal closest to the calculated 10 % of the maximum signal was used as the midpoint of five data points on each steep side of the spectral line, respectively. The five data points were used to determine the linear fit, shown in blue in Figure 3. The linear fits were used to calculate the monochromator steps corresponding to the calculated 10 % of the maximum signal on each steep side of the spectral line and Equation 1 was applied to determine the monochromator steps corresponding to the peak of the spectral line. This procedure was followed for each of the three scans performed to determine the average step position for each respective spectral line.

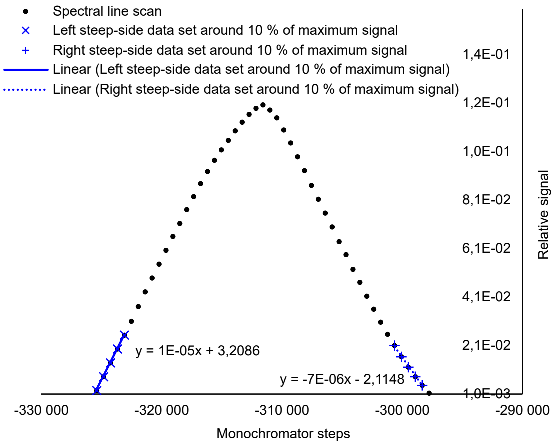

Figure 3. An example of the steep-side method and linear fits of data points around 10 % of maximum signal to determine the monochromator steps of the peak of a spectral line.

Corrections for ambient air using the NIST Enigineering Metrology Toolbox is limited to the wavelength region of 300 nm to 1 700 nm. Two of the spectral lines selected for this wavelength region, 253,7283 nm and 296,8149 nm, therefore fall outside this range. The correction applied to these two wavelengths was the refractive index determined for the ambient air as specified in the laboratory procedure for temperature, 24 °C ± 2 °C, relative humidity, 50 %RH ± 15 %RH, and an atmospheric pressure of 86 kPa at 300 nm. This approximation was applied as a best estimate and found to be sufficient as the results were within the stated uncertainty for the verification performed.

The monochromator steps were plotted against each corrected spectral line and a linear fit was applied to the data to obtain the wavelength calibration equation.

3.2. Wavelength region of 600 nm to 1 100 nm

A set of 600 g/mm gratings blazed at 800 nm was installed in the double monochromator, and an argon spectral line source was used. A large spectral area scan was performed with the monochromator from 690 nm to 990 nm in 1 nm intervals, see Figure 1, using a bandwidth of 4 nm. The spectral lines selected from this scan were, in vacuum, 696,7352 nm, 912,5471 nm and 966,0435 nm. Each of these spectral lines were scanned using a smaller wavelength interval of 0,1 nm. The scans were performed over a wavelength range of ± 5 nm of the spectral line.

The closest value of monochromator steps at the steep sides of each spectral line corresponding to 10 % of the maximum signal was determined. The largest difference between the closest value and calculated value of monochromator steps using the linear fits as in Figure 3, was approximately 36 monochromator steps. This is equal to approximately 0,025 nm, which is small in comparison with the wavelength uncertainty of ± 0,2 nm obtained.

The monochromator steps were plotted against each corrected spectral line and a linear fit was applied to the data to obtain the wavelength calibration equation.

4. Results

The wavelength calibration equation for the 200 nm to 400 nm region was found to be:

$$y(\lambda) = 288,047\lambda - 855\ 187 \tag{3}$$

where $y(\lambda)$ is the monochromator steps and λ is the wavelength in Angstrom [Å], see Figure 4. The uncertainty of measurement in wavelength was ± 0,3 nm.

The wavelength calibration equation for the 600 nm to 1 100 nm region was found to be:

$$y(\lambda) = 144,028\lambda - 1\ 003\ 276 \tag{4}$$

See Figure 5. The uncertainty of measurement in wavelength was ± 0,2 nm.

The uncertainty calculations are provided in Appendix A and Appendix B. For a more detailed description, refer to the dissertation by Rabe [5].

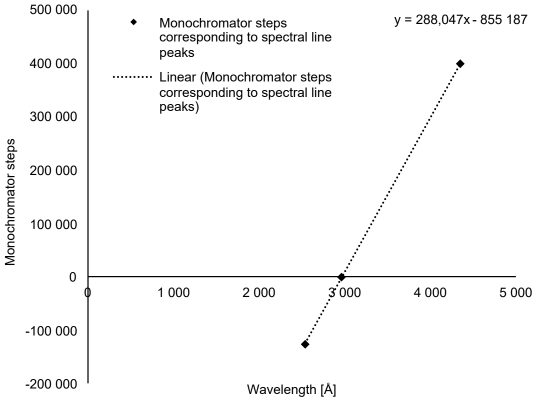

Figure 4. A plot of the monochromator steps corresponding to spectral lines peaks with a linear fit for the wavelength calibration in the region 200 nm to 400 nm.

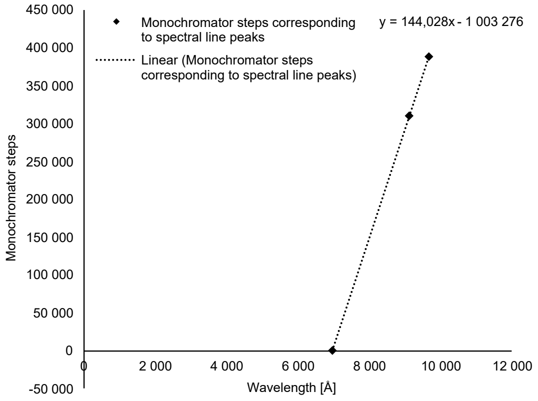

Figure 5. A plot of the monochromator steps corresponding to spectral lines peaks with a linear fit for the wavelength calibration in the region 600 nm to 1 100 nm.

5. Conclusion

As part of the characterisation of the new measurement system for spectral power responsivity of detectors implemented at NMISA, wavelength calibrations were performed in the wavelength regions of 200 nm to 400 nm and 600 nm to 1 100 nm. This was done by measuring the relevant wavelength standards for spectral lines selected from the NIST Atomic Spectra Database, and applying corrections for ambient conditions using the Engineering Metrology Toolbox of NIST. The monochromator steps corresponding to the spectral peaks measured were determined using the steep-side method. A linear plot of the spectral peaks versus the corresponding monochromator steps was used to obtain the wavelength calibration equations to be used in the respective wavelength regions when operating the monochromator. The uncertainty of measurement was calculated for each of the wavelength calibrations. The verifications performed in each wavelength region were successful when compared with the uncertainty of measurement obtained.

Appendix A. Uncertainty of measurement for the wavelength calibration in the 200 nm to 400 nm region

Appendix B. Uncertainty of measurement for the wavelength calibration in the 600 nm to 1 100 nm region

References

[1] Kostkowski H J 1997 *Reliable Spectroradiometry* (Maryland: Spectroradiometry Consulting)

[2] NIST 2019 *Atomic Spectra Database Lines Form* [Online] Available at: `https://www.nist.gov/pml/atomic-spectra-database`

[3] NIST 2004 *Engineering Metrology Toolbox* [Online] Available at: `https://emtoolbox.nist.gov/Wavelength/Edlen.asp`

[4] JCGM 2008 *JCGM 100:2008 Evaluation of measurement data — Guide to the expression of uncertainty in measurement* 1st ed

Table A1. Uncertainty of measurement calculated for the wavelength calibration in the wavelength region of 200 nm to 400 nm.

No.	Input quantity	Estimated uncertainty		Probability distribution	Coverage factor	Standard uncertainty		Sensitivity coefficient		Uncertainty contribution	
i	X_i	$u_e(x_i)$	unit		k	$u(x_i)$	unit	c_i	unit	$u_i(y)$	unit
1	Theoretical value spectral line in vacuum	1,73E-04	nm	Normal	1	1,73E-04	nm	1,00E+00		1,73E-04	nm
2	Modified Edlen equation calculation	7,39E-08	1	Normal	2	3,70E-08	1	-3,29E+03	nm/1	1,21E-04	nm
3	Laboratory temperature effect	4,00E+00	°C	Triangular	$\sqrt{6}$	1,63E+00	°C	3,53E-04	nm/°C	5,76E-04	nm
4	Laboratory humidity effect	3,00E+01	%RH	U-shaped	$\sqrt{2}$	2,12E+01	%RH	4,50E-06	nm/%RH	9,55E-05	nm
5	Laboratory air pressure effect	4,00E+00	kPa	Rectangular	$\sqrt{3}$	2,31E+00	kPa	1,17E-03	nm/kPa	2,71E-03	nm
6	Wavelength calibration equation offset	2,87E+02	steps	Normal	1	2,87E+02	steps	3,47E-04	nm/steps	9,95E-02	nm
7	Wavelength reproducibility	5,00E-03	nm	Rectangular	$\sqrt{3}$	2,89E-03	nm	1,00E+00		2,89E-03	nm
8	Mechanical resolution of monochromator	2,50E-02	nm	Rectangular	$\sqrt{3}$	1,44E-02	nm	1,00E+00		1,44E-02	nm
9	Resolution used in calibration	1,00E-01	nm	Rectangular	$\sqrt{3}$	5,77E-02	nm	1,00E+00		5,77E-02	nm
10	Repeatability	8,37E+01	steps	Normal	1	8,37E+01	steps	3,47E-04	nm/steps	2,91E-02	nm
									$u_c(y)$	1,20E-01	nm
									U (k=2)	3,00E-01	nm

Table B1. Uncertainty of measurement calculated for the wavelength calibration in the wavelength region of 600 nm to 1 100 nm.

No.	Input quantity	Estimated uncertainty		Probability distribution	Coverage factor	Standard uncertainty		Sensitivity coefficient		Uncertainty contribution	
i	X_i	$u_e(x_i)$	unit		k	$u(x_i)$	unit	c_i	unit	$u_i(y)$	unit
1	Theoretical value spectral line in vacuum	1,00E-04	nm	Normal	1	1,00E-04	nm	1,00E+00		1,00E-04	nm
2	Modified Edlen equation calculation	4,20E-08	1	Normal	2	2,10E-08	1	1,00E+00	nm/1	2,10E-08	nm
3	Laboratory temperature effect	4,00E+00	°C	Triangular	$\sqrt{6}$	1,63E+00	°C	6,81E-04	nm/°C	1,11E-03	nm
4	Laboratory humidity effect	3,00E+01	%RH	U-shaped	$\sqrt{2}$	2,12E+01	%RH	9,29E-06	nm/%RH	1,97E-04	nm
5	Laboratory air pressure effect	4,00E+00	kPa	Rectangular	$\sqrt{3}$	2,31E+00	kPa	2,26E-03	nm/kPa	5,21E-03	nm
6	Steep-side method offset	3,60E+01	steps	Normal	1	3,60E+01	steps	6,94E-04	nm/steps	2,50E-02	nm
7	Wavelength calibration equation offset	7,20E+01	steps	Normal	1	7,20E+01	steps	6,94E-04	nm/steps	5,00E-02	nm
8	Wavelength reproducibility	5,00E-03	nm	Rectangular	$\sqrt{3}$	2,89E-03	nm	1,00E+00		2,89E-03	nm
9	Mechanical resolution of monochromator	5,00E-02	nm	Rectangular	$\sqrt{3}$	2,89E-02	nm	1,00E+00		2,89E-02	nm
10	Resolution used in calibration	5,00E-02	nm	Rectangular	$\sqrt{3}$	2,89E-02	nm	1,00E+00		2,89E-02	nm
11	Repeatability	1,56E+01	steps	Normal	1	1,56E+01	steps	6,94E-04	nm/steps	1,08E-02	nm
									$u_c(y)$	7,03E-02	nm
									U (k=2)	2,00E-01	nm

[5] Rabe I 2022 *Characterisation and uncertainty of measurement analysis of a detector spectral power responsivity measurement system* Master's thesis University of Pretoria